

# A Laplace's method for series and the semiclassical analysis of epidemiological models

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## Abstract

We develop a Laplace's method to compute the asymptotic expansions of sum of sharply peaked sequences. These series arise as discretizations (Riemann sums) of integrals, whose asymptotic behaviour can be computed by the standard Laplace's method. We show that if the discretization is fine enough than the series is asymptotic to the integral, else the series is oscillatory. We apply the Laplace's method for series to the semiclassical analysis of models of population biology, with special focus on the SIS model. In this field, we show that two different and widely-used approaches to the semiclassical limit are equivalent.

**Keywords:** Laplace's method for series; asymptotic expansion; semiclassical analysis; SIS model.

## Introduction

In this paper we develop a Laplace's method to deal with series whose summand is sharply peaked about its maximum. More precisely, the main object of the paper is the asymptotic evaluation of series like

$$I(n, \alpha) = n^{\alpha-1} \sum_{k=0}^{\infty} e^{-nf(\frac{k}{n^\alpha})} g(\frac{k}{n^\alpha}), \alpha > 0, \mathbb{R}^+ \ni n \rightarrow +\infty, \quad (1)$$

for some regular enough functions  $f, g : [0, \infty[ \rightarrow \mathbb{R}$ .

The series  $I(n, \alpha)$  is actually a Riemann sum, with respect to a homogeneous partition of the positive semi-axis into subintervals of length  $1/n^\alpha$ , of the integral

$$\mathcal{I}(n) = n \int_0^\infty e^{-nf(x)} g(x) dx, \quad (2)$$

and the asymptotic behaviour of the latter integral can be computed by the (standard) Laplace's method provided it applies, see e.g. [3] [2] [16] [11].

One can expect the series to have the same asymptotic behaviour as the integral if the partition is fine enough, that is for  $\alpha$  big, while under a certain threshold the

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effects of the discretization cannot be neglected. This is indeed the case. Depending on the local nature of the global minimum of  $f$ , there is an  $\alpha^*$  below which the asymptotic of the series and of the integral do not coincide, and the series is oscillatory and even exponentially small with respect to the integral - a pictorial representation of this phenomenon can be found in Figure 1(b) at the end of Section 1 below.

For example, we will show that if  $f$  has a single global minimum point  $x_0 \neq 0$  such that  $f''(x_0) \neq 0$  and  $g(x_0) \neq 0$  then (we refer to Theorem 1 and Corollary 2 for the precise hypotheses and statement)

- if  $\alpha > \frac{1}{2}$ ,

$$I(n, \alpha) \sim \mathcal{I}(n) \sim e^{-nf(x_0)} g(x_0) \sqrt{\frac{2\pi n}{f''(x_0)}} .$$

- if  $\alpha = \frac{1}{2}$ ,

$$I(n, \frac{1}{2}) \sim e^{-nf(x_0)} g(x_0) \sqrt{\frac{2\pi n}{f''(x_0)}} \theta_3(-\sqrt{n\pi}x_0, e^{-\frac{2\pi^2}{f''(x_0)}}) ,$$

where  $\theta_3(z, q)$  is the third Jacobi theta-function [5]

- if  $\alpha < \frac{1}{2}$ ,

$$I(n, \alpha) \sim n^{\alpha-1} e^{-nf(x_0)} g(x_0) \left( e^{-\frac{f''(x_0)}{2} n^{1-2\alpha} t^2(n^\alpha x_0)} + e^{-\frac{f''(x_0)}{2} n^{1-2\alpha} (1-t(n^\alpha x_0))^2} \right) ,$$

where  $t(x) = \min\{x - \lfloor x \rfloor, \lceil x \rceil - x\}$  is the positive triangular wave of height  $\frac{1}{2}$  and period 1.

The reader may wonder whether such a seemingly natural object like  $I(n, \alpha)$  had not already been studied and well-understood in the literature. Contrary to our expectations we found few mathematical works devoted to it, the most recent being [15] [13]. Paper [15] deals with the case  $\alpha = \frac{1}{2}$  (in our notation) and its application to  $q$ -polynomials while [13] is devoted to the study of a class of hypergeometric functions defined by series that fall in the case  $\alpha = 1$ . The thorough discussion of the existing literature contained in [13] shows that the series  $I(n, \alpha)$  was never considered in the general and simple form we do here.

Contrary to the existing works on the subject, our interest does not stem from the asymptotic theory of special functions, but from a branch of applied mathematics in rapid evolution, the semiclassical limit of continuous time Markov process, in particular processes related to epidemiological models such as SIS and SIRS models [14]. The semiclassical limit of continuous time Markov process originated from the paper [6], where it was noticed that many models of population biology (or more in general skip-free continuous time Markov chains) can be solved by a method similar to the WKB method for quantum mechanics in the *semiclassical* asymptotic regime.

The semiclassical regime arises when we consider a population of large size  $n \in \mathbb{N}$  and we assume that either the probability distribution  $p_k$  is semiclassical, i.e.

$$p_k \sim e^{-nS(\frac{k}{n})} L(\frac{k}{n}) , \quad k \in \{0, 1, \dots, n\}$$

or the generating function is semiclassical, i.e.

$$\Gamma(z) \equiv \sum_{k=0}^n p(k, n) z^k \sim e^{n\Sigma(z)} \Lambda(z), \quad z > 0.$$

If one of the two hypotheses holds then, accordingly, either  $S, L$  or  $\Sigma, \Lambda$  evolve according to a pair of PDEs of the classical mechanics, a Hamilton-Jacobi equation and a related transport equation. For example, in the SIS model we consider below, these pairs of equations are either equations (24,25) or equations (26,27).

Both approaches have been used with success and it turns out that the generating function plays the role of the momentum representation in quantum mechanics [6],[4], [7], [14]. However, it was not at all clear whether the two semiclassical asymptotic regimes coincide, whether a semiclassical probability distribution implies or not a semiclassical generating function.

We will be able to answer this and other related questions analyzing the generating function by means of the Laplace's method we will have developed. The generating function is in fact a series of the kind  $I(n, \alpha = 1)$  if we set  $f(x) = S(x) - x \ln z$  and  $g(x) = L(x)\chi_{[0,1]}$ . The Laplace's method will then allow us to show that if the probability distribution is semiclassical then the generating function is semiclassical too. It will moreover allow us to compute explicitly  $\Sigma$  and  $\Lambda$ . For example  $\Sigma$  turns out to be the (restricted) Legendre-Fenchel transform of  $S$ , namely  $\Sigma(z) = \sup_{x \in [0,1]} \{-S(x) + x \ln z\}$ . Among the various consequences of these computations - see Section 2 below - the most important is probably the equivalence, under some reasonable assumptions, of the two approaches to the semiclassical limit of SIS model.

The paper is divided into two main Sections. In Section 1 we develop the Laplace's method for the series  $I(n, \alpha)$  while Section 2 is devoted to the application of Laplace's method (in the case  $\alpha = 1$ ) to the semiclassical limit of the SIS model. In Section 2 we assume that the reader has some knowledge of the classical theory of Hamilton-Jacobi equation. Finally in the concluding remarks, we comment on possible generalizations of the Laplace's method and on some open problems.

For the benefit of the reader, we end this Introduction with a summary of our main results about the asymptotic behaviour of  $I(n, \alpha)$ .

**Summary of the Asymptotic Behaviours of  $I(n, \alpha)$**  As it is customary in the Laplace's method for integrals, and essentially without losing in generality, we suppose that the function  $f$  has a single global minimum for  $x \in [0, \infty[$  and we identify two different cases, when the minimum point belongs to the open interval  $]0, \infty[$  and when the minimum point belongs to the boundary, i.e it is 0.

**Global minimum in the open interval** Assuming  $I(n, \alpha)$  converges absolutely for  $n$  big enough and that at the minimum point  $x_0$   $f''(x_0) > 0, (x_0) \neq 0$  then (for the precise hypotheses and statement we refer to Theorem 1 and Corollary

2)

$$I(n, \alpha) \sim e^{-nf(x_0)} g(x_0) \begin{cases} \sqrt{\frac{2\pi n}{f''(x_0)}}, & \text{if } \alpha > \frac{1}{2} \\ \sqrt{\frac{2\pi n}{f''(x_0)}} \theta_3(-\sqrt{n\pi} x_0, e^{-\frac{2\pi^2}{f''(x_0)}}), & \text{if } \alpha = \frac{1}{2} \\ n^{\alpha-1} \left( e^{-\frac{f''(x_0)}{2}} n^{1-2\alpha} t^2(n^\alpha x_0) + e^{-\frac{f''(x_0)}{2}} n^{1-2\alpha} (1-t(n^\alpha x_0))^2 \right), & \text{if } 0 < \alpha < \frac{1}{2} \end{cases} \quad (3)$$

where  $\theta_3(z, q)$  is the third Jacobi theta-function [5] and  $t(x) = \min\{x - \lfloor x \rfloor, \lceil x \rceil - x\}$ .

With our assumption on  $f, g$ , the standard Laplace's method for integrals [16] [11] implies that  $\mathcal{I}(n) \sim e^{-nf(x_0)} g(x_0) \sqrt{\frac{2\pi n}{f''(x_0)}}$ . Therefore after Theorem 1 we conclude that  $I(n, \alpha) \sim \mathcal{I}(n)$  if and only if  $\alpha > \frac{1}{2}$ , while if  $\alpha < \frac{1}{2}$   $I(n)$  oscillates as a consequence of the coarser discretization.

Specializing to the case  $\alpha = 1$ , in Theorem 2 we prove that  $I(n)$  admits for (locally) smooth  $f, g$  an asymptotic expansion in odd powers of  $n^{-\frac{1}{2}}$  which coincides term by term with the asymptotic expansion of the integral  $\mathcal{I}(n)$ .

**Global minimum attained at the boundary** Assuming the global minimum is attained at 0 and  $f'(0) < 0, g(0) \neq 0$  (for the precise hypotheses and statement we refer to Theorem 3) then

$$I(n, \alpha) \sim e^{-nf(0)} g(0) \begin{cases} \frac{1}{-f'(0)}, & \text{if } \alpha > 1 \\ \frac{1}{1-e^{-f'(0)}}, & \text{if } \alpha = 1 \\ n^{\alpha-1}, & \text{if } 0 < \alpha < 1 \end{cases} \quad (4)$$

Considering that by Watson's Lemma  $\mathcal{I}(n) \sim \frac{e^{-nf(0)} g(0)}{-f'(0)}$  [16],[11], then in this case the series is asymptotic to the integral  $I(n, \alpha) \sim \mathcal{I}(n)$  if and only if  $\alpha > 1$ .

Specializing to  $\alpha = 1$ , we prove in Theorem 4 that  $I(n)$  admits for (locally) smooth  $f, g$  an asymptotic expansion in powers of  $n^{-1}$ .

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## 1 Laplace's method for series

In analogy with the standard proofs of the Laplace's method for integral [3], [2], [11], [16], the main strategy of our proofs is the comparison of the series  $I(n)$  with a standard one, which is either an exponential sum

$$E(n, \alpha, \gamma) = \sum_{k \geq 0} e^{-\gamma n^{\alpha-1} k} = \frac{1 + O(e^{-\gamma n})}{1 - e^{-\gamma n^{\alpha-1}}}, \quad \gamma > 0 \quad (5)$$

or a Gaussian sum

$$Q(n, \alpha, \gamma, x_0) = \sum_{k \in \mathbb{Z}} e^{-n^{1-2\alpha} \gamma (k - n^\alpha x_0)^2}, \quad \gamma > 0. \quad (6)$$

In fact, we show that the series we consider can be reduced, up to an exponentially small relative error, to these ones. We begin therefore the Section with a list of the asymptotic behaviours of the Gaussian series for all values of  $\alpha$  (exponential sums being trivial). Even though all these Gaussian series can be written in terms of well-known Theta functions [12], the asymptotic regimes we explore here fall in general outside the ones normally considered because if we write the Gaussian sums as Theta functions then in general both the nome and the variable will depend on  $n$ .

**Lemma 1.** *The series  $Q(n, \alpha, \gamma, x_0)$  (6) has the following asymptotic behaviour depending on  $\alpha > 0$ :*

*If  $\alpha > \frac{1}{2}$  then*

$$Q(n, \alpha, \gamma, x_0) = n^{1-\alpha} \sqrt{\frac{\pi n}{\gamma}} (1 + O(e^{-\frac{2\pi}{\gamma} n^{-1+2\alpha}})) . \quad (7)$$

*If  $\alpha = \frac{1}{2}$ , then the Gaussian sum is a Jacobi theta function of fixed nome  $q = e^{-\frac{\pi^2}{\gamma}}$*

$$Q(n, \frac{1}{2}, \gamma, x_0) = \sqrt{\frac{\pi}{\gamma}} \theta_3(-\sqrt{n\pi}x_0, e^{-\frac{\pi^2}{\gamma}}) . \quad (8)$$

*Notice that it is a strictly positive periodic function of  $(\sqrt{n\pi}x_0 - \lfloor \sqrt{n\pi}x_0 \rfloor)$ .*

*If  $\alpha < \frac{1}{2}$ ,*

$$Q(n, \alpha, \gamma, x_0) = e^{-\gamma n^{1-2\alpha} t^2(n^\alpha x_0)} + e^{-\gamma n^{1-2\alpha} (1-t(n^\alpha x_0))^2} + O(e^{-\gamma n^{1-2\alpha}}) . \quad (9)$$

*where  $t(x)$  is the positive triangular wave of height  $\frac{1}{2}$  and period 1, namely*

$$t(x) = \min\{x - \lfloor x \rfloor\} . \quad (10)$$

*Proof.* We split the proof into three cases, corresponding to  $1 - 2\alpha$  negative, zero, or positive. The three must be dealt with using different techniques.

In case  $1 - 2\alpha < 0$ , the summand does not decrease fast uniformly on  $n$ . We transform the series into a tractable one by means of the Poisson summation formula, which for Gaussian series boils down to the following renowned (although slightly disguised) identity [12]

$$\sum_{k \in \mathbb{Z}} e^{-n^{1-2\alpha} \gamma (k - n^\alpha x_0)^2} = n^{1-\alpha} \sqrt{\frac{\pi n}{\gamma}} \sum_{q \in 2\pi\mathbb{Z}} e^{-\frac{n^{-1+2\alpha}}{2\gamma} q(q + \frac{2ix_0\gamma}{n^\alpha})}$$

The term  $q = 0$  is equal to  $n^{1-\alpha} \sqrt{\frac{\pi n}{\gamma}}$  while the total contribution of terms  $q \neq 0$  is easily bounded from above by considering that  $q^2 \geq q$  for  $q \geq 1$

$$\left| \sum_{q \in 2\pi\mathbb{Z}, q \neq 0} e^{-\frac{n^{-1+2\alpha}}{2\gamma} q(q + \frac{2ix_0\gamma}{n^\alpha})} \right| \leq 2 \sum_{q \in \mathbb{N} \setminus \{0\}} e^{-\frac{2\pi n^{-1+2\alpha}}{\gamma} q} = O(e^{-\frac{n^{-1+2\alpha} 2\pi}{\gamma}}) .$$

Stricter bounds can be actually given but they are irrelevant for our purpose, as this simple one is enough to prove the thesis.

The case  $\alpha = \frac{1}{2}$  follows simply from the definition of Jacobi theta functions [5].

The case  $1 - 2\alpha > 0$  is slightly more delicate. The maximum of the summand is achieved when  $n^\alpha x_0$  is closest to 0, and this term contributes as  $e^{-n^{1-2\alpha} t^2(n^\alpha x_0)}$ .

The second highest contribution is  $e^{-n^{1-2\alpha}(1-t(n^\alpha x_0))^2}$ . If  $t(n^\alpha x_0) \approx \frac{1}{2}$  then this second contribution cannot be neglected. However, all other contributions are easily bounded, as

$$Q(n, \alpha, \gamma, x_0) - e^{-n^{1-2\alpha}t^2(n^\alpha x_0)} - e^{-n^{1-2\alpha}(1-t(n^\alpha x_0))^2} \leq 2 \sum_{k \geq 1} e^{-\gamma n^{1-2\alpha}k} = O(e^{-\gamma n^{1-2\alpha}}).$$

□

Having collected the asymptotic behaviour of the standard series we need, we can now state and prove our Theorems on the Laplace's method for series.

We start with the case of the global minimum point belonging to the open interval  $]0, \infty[$ . In Theorem 1, we compute the leading asymptotic behaviour of  $I(n, \alpha)$  for a general  $\alpha$ . In Theorem 2, we specialize to the case  $\alpha = 1$  and compute the full asymptotic expansion of  $I(n, 1)$ , by showing that it coincides at all orders with the well-known asymptotic expansion of the integral  $\mathcal{I}(n)$ . We prove the latter Theorem by comparing the series and the integral by means of Euler-McLaurin formula.

**Theorem 1.** *For  $\alpha > 0$  consider the series*

$$I(n, \alpha) = n^{\alpha-1} \sum_{k=0}^{\infty} e^{-nf(\frac{k}{n^\alpha})} g(\frac{k}{n^\alpha})$$

where  $f : [0, \infty[ \rightarrow \mathbb{R} \cup \{+\infty\}$  and  $g : [0, \infty[ \rightarrow \mathbb{R}$  are such that

- (i)  $f$  has a single global minimum point  $x_0 \neq 0$  and  $f$  is twice differentiable in a neighborhood of  $x_0$  with  $f''(x_0) > 0$
- (ii)  $\exists \delta > 0$  such that  $\inf_{|x-x_0|>\delta} f(x) > f(x_0)$
- (iii)  $g$  is globally bounded and continuous in a neighborhood of  $x_0$
- (iv)  $f$  is bounded from below by a function, increasing on the open interval  $[x_0, \infty[$  and such that  $F(x_0) = f(x_0)$  and  $\sum_{k=0}^{\infty} e^{-n_0 F(k)} < \infty$  for some  $n_0 > 0$ .

If  $\alpha > \frac{1}{2}$  then

$$I(n, \alpha) = \sqrt{\frac{2\pi n}{f''(x_0)}} e^{-nf(x_0)} (g(x_0) + O(n^{-\beta})), \forall 0 < \beta < \frac{1}{2}. \quad (11)$$

If  $\alpha = \frac{1}{2}$  then

$$I(n, \frac{1}{2}) = e^{-nf(x_0)} \sqrt{\frac{2\pi n}{f''(x_0)}} g(x_0) \times \theta_3 \left( -\sqrt{n}\pi x_0, e^{-\frac{2\pi^2}{f''(x_0)}} \right) (1 + O(n^{-\beta})), \forall 0 < \beta < \frac{1}{2}. \quad (12)$$

If  $\alpha < \frac{1}{2}$  then

$$I(n, \alpha) = n^{\alpha-1} e^{-nf(x_0)} g(x_0) P \left( n, \alpha, \frac{f''(x_0)}{2} (1 + O(n^{-\beta})), x_0 \right), \forall 0 < \beta < \alpha \quad (13)$$

where  $P(n, \alpha, \gamma, x_0)$  is the oscillating sequence

$$P(n, \alpha, \gamma, x_0) = e^{-\gamma n^{1-2\alpha} t^2(n^\alpha x_0)} + e^{-\gamma n^{1-2\alpha} (1-t(n^\alpha x_0))^2}, \quad (14)$$

with  $t(x) = \min\{x - \lfloor x \rfloor, \lceil x \rceil - x\}$ .

*Proof.* If we multiply the series by  $e^{nf(x_0)}$  we reduce to the case  $f(x_0) = F(x_0) = 0$ , which we assume to hold. Before we start proving the asymptotic result, we notice that  $|I(n, \alpha)| \leq n^\alpha C$  for some  $C < \infty$  (for simplicity we assume that  $\sum_k e^{-n_0 F(k)}$  converges for  $n_0 = 1$ ; the results are independent on the choice of  $n_0$  but this choice simplifies the notation). In fact due to assumption (iii,iv)

$$\sum_{k=0}^{\infty} e^{-nf(\frac{k}{n})} |g(\frac{k}{n})| \leq \sup_x |g(x)| \sum_x e^{-nF(\frac{k}{n^\alpha})} < (n^\alpha + 1) \sup_x |g(x)| (x_0 + \sum_{k=\lceil n^\alpha x_0 \rceil}^{\infty} e^{-F(k)}).$$

The latter inequality stems from the fact that  $e^{-F}$  is a decreasing function on  $[x_0, \infty)$ .

The strategy of the proof goes as follows. First I) we show that terms not sufficiently close to the maximum are exponentially suppressed, then II) we show that the remaining terms are asymptotic to the Gaussian sum  $Q(n, \alpha, \frac{f''(x_0)}{2}, x_0)$  up to the stated error.

I) For the hypotheses (i,ii) on  $f$  it follows if  $\delta > 0$  is small enough there exists a  $0 < \mu \leq f''(x_0)$  such that  $f(x) \geq \mu\delta$  for all  $|x - x_0| \geq \delta$ .

Then trivially

$$nf(\frac{k}{n^\alpha}) \geq (n-1)\mu\delta^2 + f(\frac{k}{n^\alpha}),$$

and

$$\sum_{|k - n^\alpha x_0| \geq n^\alpha \delta} e^{-nf(\frac{k}{n^\alpha})} g(\frac{k}{n^\alpha}) \leq e^{-\mu(n-1)\delta^2} \sum_{k=0}^{\infty} e^{-nf(\frac{k}{n^\alpha})} g(\frac{k}{n^\alpha}) \leq n^\alpha e^{-\mu n \delta^2} C.$$

Therefore, if  $\delta$  is fixed or it tends to 0 slowly enough,  $\delta = n^{-\beta}$  with  $0 < \beta < \frac{1}{2}$ , the total contribution of all terms away from  $n^\alpha x_0$  is (sub-)exponentially small.

The same principle holds also for Gaussian series  $Q(n, \alpha, \gamma, x_0)$ ,  $\gamma > 0$ , the contribution all terms away from  $n^\alpha x_0$  is exponentially small - we can actually give a slightly better bound -

$$Q(n, \alpha, \gamma, x_0) - \sum_{|k - n^\alpha x_0| \geq n^\alpha \delta} e^{-n^{1-2\alpha}(k - n^\alpha x_0)^2} \leq 2 \frac{e^{-\gamma n \delta^2}}{1 - e^{-\gamma n^{1-2\alpha}}} \leq C' n^\alpha e^{-\gamma n \delta^2}.$$

II) To prove the thesis, we have now to compare the truncated series  $I(n, \alpha)$  with the truncated Gaussian series  $Q(n, \alpha, \frac{f''(x_0)}{2}, x_0)$ , whose asymptotic behaviour is listed in Lemma 1. This is done by Taylor expansion. In fact, for  $x \approx x_0$ ,  $f$  is twice differentiable and  $g$  continuous, thus  $f(x) = (\frac{f''(x_0)}{2} + o(\delta))(x - x_0)^2$ ,  $g(x) = g(x_0) + o(\delta)$ .

Therefore, for any  $\alpha$  we have

$$I(n, \alpha) = Q\left(n, \alpha, \frac{f''(x_0)}{2}(1 + o(\delta)), x_0\right) (g(x_0)(1 + o(\delta)) + \text{error terms}).$$

where the error terms are, i) the difference between  $I(n, \alpha)$  and its truncation which is less than  $Cn^\alpha e^{-\mu n\delta^2}$ , and ii) the difference between the Gaussian series and its truncations, which is less than  $C'n^\alpha e^{-\frac{f''(x_0)}{2}n\delta^2}$ . Since  $\mu \leq \frac{f''(x_0)}{2}$  then the error terms are  $O(n^\alpha e^{-\mu n\delta^2})$ .

If  $\alpha > \frac{1}{2}$ , then for any  $\beta < \frac{1}{2}$

$$I(n, \alpha) = \sqrt{\frac{2\pi n}{f''(x_0)(1 + o(n^{-\beta}))}} (g(x_0)(1 + o(n^{-\beta})) + O(n^\alpha e^{-\frac{f''(x_0)}{2}n^{1-2\beta}})) = \sqrt{\frac{2\pi n}{f''(x_0)}} (g(x_0)(1 + o(n^{-\beta})) ,$$

which proves the thesis.

For  $\alpha = \frac{1}{2}$ , the same consideration holds, only the dominant term is different.

For  $\alpha < \frac{1}{2}$  some more care is needed. This is because the asymptotic behaviour of the Gaussian sum (9) oscillates between 1 and  $\exp\{-n^{1-2\alpha} \frac{f''(x_0)}{2}(1 + o(\delta))\}$ , which is exponentially small. and thus potentially comparable with the error terms. However if we let  $\delta = n^{-\beta}$  with  $0 < \beta < \alpha$  then all error terms are subdominant with respect to  $\exp\{-n^{1-2\alpha} \frac{f''(x_0)}{2}(1 + o(\delta))\}$  and

$$I(n, \alpha) = P\left(n, \alpha, \frac{f''(x_0)}{2}(1 + o(n^{-\beta})), x_0\right) .$$

□

**Remark.** Hypothesis (iv) of Theorem 1 can be relaxed and substituted by any hypothesis assuring that  $|I(n, \alpha)|$  does not grow exponentially with  $n$ . However, the hypothesis we choose is not very restrictive since it holds for any function  $f$  such that  $|f|(x) \geq c \log x$  for some  $c > 0$  and for  $x$  big enough.

**Corollary 1.** Let  $f, g$  be measurable functions satisfying the same hypotheses of Theorem 1. If  $\alpha > \frac{1}{2}$  and  $g(x_0) \neq 0$  then  $I(n, \alpha) \sim \mathcal{I}(n) \equiv n \int_0^\infty e^{-nf(x)} g(x) dx$ .

*Proof.* If the integral would converge then the thesis follows from the standard Laplace's method for integrals [16], which states that  $\mathcal{I}(n) \sim \sqrt{\frac{2\pi n}{f''(x_0)}} g(x_0)$ .

The integral do converge. In fact,  $e^{-nF(x)}$  is measurable because  $F$  is monotone. Therefore  $\mathcal{I} \leq \sup_x |g(x)| \int_0^\infty e^{-nF(x)} dx$  which is dominated by  $\sum_{k=0}^\infty e^{-nF(\frac{k}{n})}$  because  $e^{-nF}$  is a decreasing function. □

**Corollary 2.** Let  $f, g$  satisfy all hypotheses of Theorem 1 and, in addition to that, let us assume that  $g(x_0) \neq 0$ . Then

$$I(n, \alpha) \sim e^{-nf(x_0)} g(x_0) \begin{cases} \sqrt{\frac{2\pi n}{f''(x_0)}} , & \text{if } \alpha > \frac{1}{2} \\ \sqrt{\frac{2\pi n}{f''(x_0)}} \theta_3(-\sqrt{n\pi} x_0, e^{-\frac{2\pi^2}{f''(x_0)}}) , & \text{if } \alpha = \frac{1}{2} \\ n^{\alpha-1} P(n, \alpha, \frac{f''(x_0)}{2}, x_0) , & \text{if } \frac{1}{3} < \alpha < \frac{1}{2} \end{cases} .$$

If  $\alpha \leq \frac{1}{3}$  then

$$\lim_{n \rightarrow \infty} e^{nf(x_0)} n^{\alpha-1} (I(n, \alpha) - P(n, \alpha, \frac{f''(x_0)}{2}, x_0)) = 0$$



*Proof.* Again, we assume  $f(x_0) = 0$ .

For  $\alpha \geq \frac{1}{2}$  the statement is trivial to verify after (1, 12) of Theorem 1.

In case  $\alpha < \frac{1}{2}$ , then after (13) we have, for any  $0 < \beta < \alpha$ ,

$$\frac{I(n, \alpha)}{g(x_0)n^{\alpha-1}P(n, \alpha, \frac{f''(x_0)}{2}, x_0)} = e^{-\frac{f''(x_0)}{2}t^2(n^\alpha x_0)O(n^{1-2\alpha-\beta})} + e^{-\frac{f''(x_0)}{2}(1-t(n^\alpha x_0))^2O(n^{1-2\alpha-\beta})}.$$

If  $\alpha > \frac{1}{3}$  then  $1 - 2\alpha - \beta$  can be chosen to be negative and therefore the limit of the ratio is 1.

If else  $\alpha \leq \frac{1}{3}$ ,  $1 - 2\alpha - \beta$  cannot be chosen negative and we cannot conclude that the limit of the ratio is 1. However, the weaker statement holds

$$\lim_{n \rightarrow \infty} e^{nf(x_0)} n^{\alpha-1} (I(n, \alpha) - P(n, \alpha, \frac{f''(x_0)}{2}, x_0)) = 0.$$

In fact, fix  $c > 0$ ,  $\varepsilon < \beta < \alpha$ . For any sequence  $n \rightarrow \infty$ , let  $n_l$  the subsequence such that  $t^2(n_l^\alpha x_0) \geq cn_l^{2\alpha-1+\varepsilon}$  and  $n_m$  the complementary subsequence. We prove that for both subsequences the difference tend to 0.

For  $l \rightarrow \infty$  both  $n_l^{\alpha-1}(I(n_l, \alpha))$  and  $n_l^{\alpha-1}P(n_l, \alpha, \frac{f''(x_0)}{2}, x_0)$  go to 0 as  $e^{-c\frac{f''(x_0)}{2}n_l^\varepsilon}$ , so their difference. Conversely, for  $m \rightarrow \infty$  then, by above formula,

$$\frac{I(n_m, \alpha)}{g(x_0)n_m^{\alpha-1}P(n_m, \alpha, \frac{f''(x_0)}{2}, x_0)} \rightarrow 1.$$

□

We now assess the complete asymptotic expansion of  $I(n)$ .

**Theorem 2.** *Consider the series*

$$I(n) = \sum_{k=0}^{\infty} e^{-nf(\frac{k}{n})} g(\frac{k}{n})$$

where  $f, g$  are measurable functions satisfying the same hypotheses of Theorem 1, and in addition to them, there exists an  $m \geq 0$  such that

(i)  $f$  has  $m + 2$  continuous derivatives in a neighborhood of  $x_0$

(ii)  $g$  has  $m + 1$  continuous derivatives in a neighborhood of  $x_0$

then

$$e^{nf(x_0)} (I(n, \alpha) - n \int_0^1 e^{-nf(x)} g(x) dx) = o(n^{-\lfloor \frac{m}{2} \rfloor + \frac{1}{2}}) \quad (15)$$

which, given the well-known [16] [11] asymptotic expansion of  $\mathcal{I}(n)$ , implies that

$$I(n) = \sqrt{\frac{2n\pi}{f''(x_0)}} e^{-nf(x_0)} \left( g(x_0) + \sum_{l=1}^{\lfloor \frac{m}{2} \rfloor} a_l n^{-l} + o(n^{-m}) \right) \quad (16)$$

where  $a_l, l = 1, \dots, m$  depends on the first  $l + 2, l$  derivatives of  $f, g$  at  $x_0$ .

*Proof.* As usual, we suppose  $f(x_0) = 0$ .

As was shown at the beginning of the proof of Theorem 1, for  $n$  big enough  $|I(n, 1)| \leq nC$  for some  $C < \infty$ . The series thus eventually converges.

Since the total contributions of terms such that  $|k - nx_0| > nc$  for a fixed  $c > 0$  are negligible, for sake of simplicity we truncate the series at  $k = nn_0$  for some fixed  $\mathbb{N} \ni n_0 > x_0$ .

For the same reason, without losing generality, we also assume that  $f, g$  have  $m + 2, m + 1$  continuous derivative in the whole segment  $[0, n_0]$ .

To prove the Theorem we use Euler(-McLaurin) summation formula, according to which (see e.g. [1]) for any (integrable) function  $h$  with  $2p$  (resp.  $2p+1$ ) continuous derivatives the following formula holds

$$\sum_{k=0}^m h(k) = \int_0^n h(y) dy + \frac{h(n) - h(0)}{2} - \sum_{k=1}^p \frac{B_{2k}}{(2k)!} (h^{(2k-1)}(m) - h^{(2k-1)}(0)) + R \quad (17)$$

$$R = C_{2p} \int_0^m B_{2p}(y) h^{(2p)}(y) dy = C_{2p+1} \int_0^m B_{2p+1}(y) h^{(2p)}(y) dy.$$

Here  $B_{2k}$  is the  $2k$ -th Bernoulli number,  $B_j(y)$  is the  $j$ -th periodic Bernoulli function, which is a  $j - 2$  times differentiable periodic function of period 1 and finally  $C_j$  is some universal constant.

We apply the formula to  $h(y) = e^{-nf(y/n)} g(y/n)$  and  $m = nn_0$  to get

$$I(n) = n \int_0^{n_0} e^{-nf(x)} g(x) dx + \text{remainder}$$

where the remainder is made of contribution from the evaluation at the endpoint of the interval -which are discarded because exponentially small- and the term  $R$ , involving the integral of  $h^{(m+1)}$  as by hypothesis  $h$  has  $m + 1$  continuous derivatives.

It is well-known (see e.g. [16]) that for  $f \in C^{m+2}$  and  $g \in C^m$ , the integral admits the asymptotic expansion

$$n \int_0^{n_0} e^{-nf(x)} g(x) dx = \sqrt{\frac{\pi n}{f''(x_0)}} \left( g(x_0) + \sum_{l=1}^{\lfloor \frac{m}{2} \rfloor} a_l n^{-l} + o(n^{-\lfloor \frac{m}{2} \rfloor}) \right),$$

To prove the thesis it is therefore sufficient to prove that the term  $R$  is  $o(n^{-\lfloor \frac{m}{2} \rfloor + \frac{1}{2}})$ .

To establish this we first recognize that

$$\begin{aligned} \frac{\partial^{m+1}}{\partial x^{m+1}} (e^{-nf(y/n)} g(y/n)) &= e^{-nf(y/n)} \left( \sum_{k=0}^{\lfloor \frac{m+1}{2} \rfloor} n^{-l} (f'(y/n))^{m-2l} Q_{l,k}(f, g) + \right. \\ &\quad \left. \sum_{l > \lfloor \frac{m+1}{2} \rfloor}^m n^{-l} Q_{l,k}(f, g) \right) \end{aligned}$$

where  $Q_{m,k}(f, g)$  is a polynomial of  $f, g$  and their first  $k + 1, k$  derivatives, evaluated at  $y/n$ .

The term  $R$  is thus

$$R = n \int_0^{n_0} B_m(xn) e^{-nf(x)} \left( \sum_{k=0}^{\lfloor \frac{m}{2} \rfloor} n^{-l} (f'(x))^{m-2l} Q_{l,k}(f(x), g(x)) + \sum_{l > \lfloor \frac{m}{2} \rfloor}^m n^{-l} Q_{l,k}(f(x), g(x)) \right).$$

We notice that  $f'(x_0) = 0$  ( $x_0$  is a minimum for  $f$ ), so that  $(f'(x))^{m-2l} Q_{l,k}(f(x), g(x)) = (x - x_0)^{m-2l} r_l(x)$  for some continuous function  $r_l$ .

Since  $n \int_0^{n_0} e^{-nf(x)} g(x) (x - x_0)^{m-2l} r_l(x) = O(n^{\frac{1-m}{2}})$  (see [11]), then simple power counting shows that  $R = O(n^{-\lfloor \frac{m}{2} \rfloor})$ . This proves the thesis.  $\square$

**Corollary 3.** *If  $f, g$  satisfy the hypotheses of Theorem 2 and in addition they are smooth in the neighborhood of the unique global minimum point  $x_0$  of  $f$ , then  $I(n)$  admits an asymptotic expansion in odd (negative) powers of  $n^{\frac{1}{2}}$  that coincides with the asymptotic expansion of  $\mathcal{I}(n)$ .*

We turn now our attention to the asymptotic evaluation of  $I(n, \alpha)$  when the global minimum point is 0. In Theorem 3 we deal with the leading asymptotic behaviour of  $I(n, \alpha)$  for general  $\alpha$ , and in Theorem 4 we compute the full asymptotic expansion in case  $\alpha = 1$ . For convenience we prove the two Theorems together.

**Theorem 3.** *For  $\alpha > 0$  consider the series*

$$I(n, \alpha) = n^{\alpha-1} \sum_{k=0}^{\infty} e^{-nf(\frac{k}{n^\alpha})} g(\frac{k}{n^\alpha})$$

where  $f : [0, \infty[ \rightarrow \mathbb{R} \cup \{+\infty\}$  and  $g : [0, \infty[ \rightarrow \mathbb{R}$  are such that

- (i)  $f$  has a single global minimum at  $x = 0$
- (ii) it is differentiable in a neighborhood of 0 with  $f'(0) > 0$
- (iii)  $g$  is globally bounded and continuous in a neighborhood of  $x_0$
- (iv)  $f$  is bounded from below by a function, increasing on the open interval  $[x_0, \infty[$  and such that  $F(x_0) = f(x_0)$  and  $\sum_{k=0}^{\infty} e^{-n_0 F(k)} < \infty$  for some  $n_0 > 0$ .

then

$$I(n, \alpha) = \frac{1}{-f'(x_0)} e^{-nf(x_0)} (g(x_0) + O(n^{-\beta})), \quad \forall \beta < 1. \quad (18)$$

if  $\alpha > 1$ .

If  $\alpha = 1$  then

$$I(n) = \frac{e^{-nf(0)}}{1 - e^{-f'(0)}} (g(0) + O(n^{-\beta})), \quad \forall \beta < 1. \quad (19)$$

If  $\alpha < 1$  then

$$I(n, \alpha) = n^{\alpha-1} e^{-nf(x_0)} g(x_0) (1 + O(n^{-\beta})), \quad \forall \beta < 1. \quad (20)$$

**Corollary 4.** *Let  $f, g$  be measurable functions satisfying the same hypotheses of Theorem 3. If  $\alpha > 1$  and  $g(x_0) \neq 0$  then  $I(n, \alpha) \sim \mathcal{I}(n) \equiv n \int_0^\infty e^{-nf(x)} g(x) dx$ .*

*Proof.* As was shown in the proof of Corollary 1  $\mathcal{I}(n)$  converges for  $n$  big enough. Therefore the standard Watson's Lemma [16] (or Laplace's method) applies and  $\mathcal{I}(n) \sim \frac{1}{-f'(x_0)} e^{-nf(x_0)} g(x_0)$   $\square$

**Theorem 4.** *Consider the series*

$$I(n) = \sum_{k=0}^{\infty} e^{-nf(\frac{k}{n})} g(\frac{k}{n})$$

where  $f, g$  satisfy the same hypotheses as in Theorem 1, and in addition to them, there exists an  $m \geq 0$  such that

- (i)  $f$  has  $m+1$  continuous derivatives in a (right-)neighborhood of 0
- (ii)  $g$  has  $m$  continuous derivatives in a (right-)neighborhood of 0

then

$$I(n) = \frac{e^{-nf(0)}}{1 - e^{-f'(0)}} \left( g(0) + \sum_{l=1}^m a_l n^{-l} + o(n^{-m}) \right) \quad (21)$$

where

$$a_l = \sum_{j=0}^{m+1} b_j^l \chi_j(f'(0)) . \quad (22)$$

Here  $\chi_j(\gamma) = \sum_{k \geq 0} e^{-\gamma k} k^j$  (a special case of the Hurwitz-Lerch transcendent [5]) and  $b_j^l$  is the coefficient of the term  $k^j n^{-l}$  in the expansion of  $e^{nf(0) + f'(0)k} e^{-nf(\frac{k}{n})} g(\frac{k}{n})$  in power series of  $n^{-1}$ .

**Proof of Theorem 3 and Theorem 4** Multiplying the series by  $e^{nf(0)}$  we can reduce to the case  $f(0) = 0$ , which we assume to hold.

As it was shown at the beginning of the proof of Theorem 1, for  $n$  big enough  $|I(n, \alpha)| \leq n^\alpha C$  for some  $C < \infty$ .

For the hypotheses (i,ii) on  $f$  it follows that if  $\delta > 0$  is small enough there exists a  $0 < \mu \leq f(0)$  such that  $f(x) \geq \mu\delta$  for all  $x \geq \delta$ . Therefore

$$\sum_{|k| \geq n^\alpha \delta} e^{-nf(\frac{k}{n})} g(\frac{k}{n}) \leq n^\alpha e^{-\mu n \delta} C .$$

If  $\delta$  is fixed or  $\delta = n^{-\beta}$  with  $0 < \beta < 1$ , then the total contribution of all terms for  $k \geq n^\alpha \delta$  is exponentially small. The same principle holds also for the exponential series  $E(n, \alpha, \gamma)$  (5) which is just a special case of  $I(n, \alpha)$  with  $f(x) = \gamma x, g(x) = 1$ .

As in the proof of Theorem 1, we compare, the truncated  $I(n, \alpha)$  with the exponential series. Since  $f \in C^1$  for  $x \leq \delta$  with  $\delta$  small enough and  $g$  is continuous then  $f(x) = f'(0)(1 + o(\delta))x, g(x) = g(0) + o(\delta)$ . Therefore, for any  $\alpha > 0$  and  $\beta < 1$  if we set  $\delta = n^{-\beta}$  we get

$$I(n, \alpha) = E(n, \alpha, f'(x_0)(1 + o(n^{-\beta}))) (g(x_0) + o(n^{-\beta})) + \text{error terms} .$$

The error terms come from the truncation of  $I(n, \alpha)$  and  $E(n, \alpha, \gamma)$  and are all exponentially small provided  $\beta < 1$ . This proves the thesis of Theorem 3.

Next we analyze case  $\alpha = 1$  further to prove the asymptotic expansion.

We expand  $e^{f'(0)k} e^{-nf(\frac{k}{n})} g(\frac{k}{n})$  in power series of  $n^{-1}$  up to  $n^{-m}$ . This is possible as long as  $\delta$  is chosen such that  $n\delta^2 \rightarrow 0$  if  $n \rightarrow \infty$ , a condition assuring that  $\sum_{l=2}^{m+1} f^{(l)}(0) \frac{k^l}{n^{l-1}}$  is small. If we do the expansion we obtain

$$e^{-nf(\frac{k}{n})} g(\frac{k}{n}) = e^{-f'(0)k} \left( g(0) + \left( \sum_{l=1}^m n^{-l} \sum_{j=0}^{m+1} b_j^l k^j \right) + R_m(k) n^{-m} o(\delta) \right)$$

for some  $b_j^l$  depending on the first  $l+1$ ,  $l$  derivatives of  $f, g$  at 0, and some polynomial  $R_m(k)$ . Since

$$\sum_{k < n\delta} e^{-f'(0)k} k^j = e^{-nf'(0)} (\chi_j(f'(0)) + O(e^{-n\delta})) ,$$

then

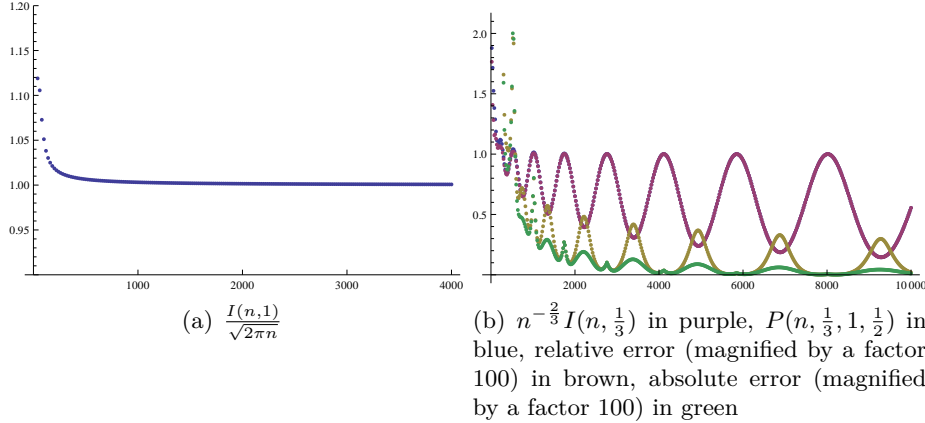
$$\sum_{k < n\delta} e^{-nf(\frac{k}{n})} g(\frac{k}{n}) = e^{-f'(0)k} \left( g(0) + \left( \sum_{l=1}^m n^{-l} \sum_{j=0}^{m+1} b_j^l \chi_j(f'(0)) \right) + n^{-m} o(\delta) \right) .$$

## A Numerical Example

We consider the series  $I(n, \alpha)$  for functions  $f(x) = \frac{1}{16} - x^2 + 2x^3 - x^4$  if  $x \in [0, 1]$ ,  $+\infty$  otherwise, and  $g(x) = 1$ .

Functions  $f, g$  satisfy the hypotheses of Theorem 1. The global minimum point of  $f$  is  $\frac{1}{2}$  and  $f(\frac{1}{2}) = 0, f''(\frac{1}{2}) = 1$ .

Below we plot  $I(n, 1)$  and  $I(n, \frac{1}{3})$  against their asymptotics, namely  $\sqrt{2\pi n}$  and  $n^{\frac{2}{3}} P(n, \frac{1}{3}, \frac{1}{2}, \frac{1}{2})$  where  $P$  is defined by formula (14).

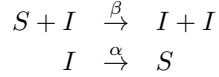


From Plot 1(b), one can see that sequence of the relative errors  $\frac{I(n, \frac{1}{3})}{P(n, \frac{1}{3})} - 1$  has a peak corresponding to any local minimum of  $P(n, \frac{1}{3})$ . These peaks prevent this sequence to tend to 0. Conversely the absolute error tends to 0. Both phenomena were predicted in the Corollary 2 and its proof.

## 2 Semiclassical Generating Functions of SIS models

In the present Section we apply the Laplace's method for sums to study the semiclassical limit of models of population biology. For sake of definiteness and as a concrete example, we stick to the SIS model, even though our considerations can be extended with few or no modifications at all to many other models of population biology admitting a semiclassical limit, such as the ones considered in [6] [4] [7] [14]

The SIS model is an epidemiological model of propagation of a disease. It may be represented by the following reaction scheme for a population of fixed size  $n$



for the stochastic variables  $I$  (infected) and  $S = n - I$  (susceptible). Here  $\beta$  is the infection rate and  $\alpha$  the recovery rate. Loosely speaking, the scheme simply indicates that a susceptible person  $S$  can get infected interacting with an infected persons  $I$  with rate  $\beta$  while an infected person  $I$  can naturally recover with rate  $\alpha$ .

Strictly speaking it indicates that the probability distribution  $p_k$  of  $k$  individuals being infected evolves with time according to the following linear equation (continuous time Markov chain or Master equation)

$$\dot{p}_k = \frac{\beta}{N}(k-1)(N-(k-1))p_{k-1} + \alpha(k+1)p_k - \left(\frac{\beta}{N}k(N-k) + \alpha k\right)p_{k+1}. \quad (23)$$

A simple (formal) computation [14] shows that if we consider a semiclassical probability distribution

$$p_k \sim c_n e^{-nS(\frac{k}{n})} L\left(\frac{k}{n}\right),$$

then, discarding higher order contribution  $O(1/n)$ ,  $S$  and  $L$  evolves according to a pair of PDEs of classical mechanics

$$S_t + H(x, S_x) = 0, \quad H(x, q) = -\alpha x(e^q - 1) + \beta x(x - 1)(e^{-q} - 1) \quad (24)$$

$$L_t + \partial_q H(x, q)|_{q=S_x} L_x + \left(\frac{1}{2}\partial_q^2 H(x, q)|_{q=S_x} S_{xx} + \partial_q \partial_x H(x, q)|_{q=S_x}\right) L = 0 \quad (25)$$

Equation (24) is the Hamilton-Jacobi equation, equation (25) is a transport equation. They both can be solved via the method of characteristics [9].

A similar (formal) computations [14] shows that also if the generating function is semi-classical

$$\Gamma(z) = \sum_{k=0}^n p_k z^k \sim d_n e^{n\Sigma(z)} \Lambda(z)$$

then its evolution is described up to  $O(1/n)$  correction by a (different) pair of Hamilton-Jacobi and transport equations

$$\Sigma_t + \Theta(z, \Sigma_z) = 0, \quad \Theta(z, q) = -(\beta z - \alpha)(z - 1)q + \beta z^2(z - 1)q^2 \quad (26)$$

$$\Lambda_t + \partial_q \Theta(z, q)|_{q=\Sigma_z} \Lambda_z + \left(\frac{1}{2}\partial_q^2 \Theta(z, q)|_{q=\Sigma_z} \Sigma_{zz} + \beta(-z + z^2)\Sigma_z\right) \Lambda = 0 \quad (27)$$

Both approaches to the semiclassical limit of systems of population biology have been used with success within the physical literature, see e.g. [6] [4] [7] [14]; depending on the specific problem they offer different advantages. The generating function is often useful as it seems to play the role of the momentum-representation in quantum mechanics [6]. Currently we are studying the long-time behaviour of the semiclassical approximation and the generating function turns out to be extremely useful to overcome the singularities that the general solution to Hamilton-Jacobi develops [10].

However, there was so far no proof that the two approaches are equivalent, in the sense that they apply to the same asymptotic regime, or in cruder words there was no proof that a semiclassical probability distribution implies a semiclassical generating function. It was even unknown whether the semiclassical equations, which are nonlinear, preserve the total probability.

After our Theorems on the Laplace's method for sums, we can prove that the two approaches are equivalent and that the total probability is conserved. We can thus furnish a *minimal mathematical (kynematical) foundation* for the semiclassical dynamics of the SIS model, by a method that is valid for all other equation of population biology (Markov processes) that allows a similar semiclassical limit.

Our main results are as follows

- First we show that if  $p_k$  is semiclassical then also  $\Gamma(z)$  is semiclassical and we compute explicitly  $\Sigma$  and  $\Lambda$ .  $\Sigma$  turns out to be the (restricted) Legendre-Fenchel transform of  $S$ . Theorem 5.
- Then we show that the  $\Sigma, \Lambda$  we obtained satisfy the semiclassical PDEs (26,27) provided  $S, L$  satisfy the semiclassical PDEs (24,25). Theorem 6.
- Eventually we show, using the semiclassical dynamics of the generating function, that the total probability is asymptotically conserved. We prove that

$$\sum_{k=0}^n e^{-nS(\frac{k}{n}, t)} L(\frac{k}{n}, t) \sim \sum_{k=0}^n e^{-nS(\frac{k}{n}, 0)} L(\frac{k}{n}, 0)$$

if  $S, L$  satisfy (24,25). Theorem 7.

We warn the reader that the proofs of Theorem 6 and Theorem 7 require some knowledge of the method of characteristics for the solution of Hamilton-Jacobi equations.

**Theorem 5.** *Let  $p_k = c_n e^{-S(\frac{k}{n})} L(\frac{k}{n})$  be a semiclassical probability distribution, where*

- $S : [0, 1] \rightarrow \mathbb{R} \cup \{+\infty\}$  *is a continuous function, twice differentiable on  $]0, 1[$ , and with a single minimum at  $x_0 \in ]0, 1[$  and such that  $S''(x) \neq 0, \forall x \in ]0, 1[$ .*
- $L : [0, 1] \rightarrow \mathbb{R}$  *is a never vanishing differentiable function.*

*and let  $\Gamma(z, n)$  its generating function.*

*Then for any  $z > 0$*

$$\Sigma(z) \equiv \lim_{n \rightarrow \infty} \frac{\ln \Gamma(z, n)}{n} = \sup_{x \in [0, 1]} \{-S(x) + x \ln z\} \quad (28)$$

$\Sigma$  *is thus the (restricted) Legendre-Fenchel transform of  $S$  evaluated at  $\ln z$  [8].*

Moreover, for any  $e^{S'(0)} < z < e^{S'(1)}$  let  $x(z)$  be the unique solution of  $f'(x) = \ln z$ . Then

$$\Gamma(z) \sim c_n e^{n\Sigma(z)} \begin{cases} \frac{1}{1 - \exp(-S'(1) + \log z)} L(1), & \text{if } z > e^{S'(1)} \\ \sqrt{\frac{\pi n}{2S''(1)}} L(1), & \text{if } z = e^{S'(1)} \\ \sqrt{\frac{2\pi n}{S''(x(z))}} L(x(z)), & e^{S'(0)} < z < e^{S'(1)} \\ \sqrt{\frac{\pi n}{2S''(0)}} L(0), & \text{if } z = e^{S'(0)} \\ \frac{1}{1 - \exp(-S'(0) + \log z)} L(0), & \text{if } z < e^{S'(0)} \end{cases} \quad (29)$$

In particular for  $e^{S'(0)} < z < e^{S'(1)}$  then

$$\Gamma(z) \sim \sqrt{2\pi n} e^{n\Sigma(z)} \Lambda(z) \text{ with } \Lambda(z) = \frac{L(x(z))}{\sqrt{S''(x(z))}} \quad (30)$$

*Proof.* The Theorem is a corollary of Theorems 2 and 4) applied to the generating function by noticing that  $\Gamma(z) = \sum_k^n e^{-n\tilde{S}(\frac{k}{n})} L(\frac{k}{n})$  where  $\tilde{S}(x) = S(x) - x \ln z$ .

The only two cases not treated explicitly in the above mentioned Theorems are when  $z = e^{S'(0)}$  or  $z = e^{S'(1)}$ . Here the maximum of the summand is achieved at the boundary, where the first derivative (but not the second) vanishes. It is easily seen that this case is analogous to the one treated in Theorem 2, the only difference being a  $\frac{1}{2}$  factor.  $\square$

**Corollary 5.** Let  $p_k = c_n e^{-S(\frac{k}{n})} L(\frac{k}{n})$  where  $S, L$  satisfies all hypotheses of Theorem 5. Then

$$\sum_{k=0}^n p_k \sim c_n \sqrt{\frac{\pi n}{S''(x_0)}} e^{-nS(x_0)} L(x_0) \quad (31)$$

where  $x_0$  is the unique global minimum point of  $S$ .

**Remark.** Since  $\Sigma$  is the (restricted) Legendre-Fenchel transform (28) then its second derivative has a jump at  $z = e^{S'(0)}, z = e^{S'(1)}$ .

Hypotheses of the Theorem can be relaxed. In fact, one can show that  $\Sigma$  exists and it the Legendre-Fenchel transform of  $S$  even if  $S''$  vanishes or  $S$  is not twice differentiable, provided  $S$  is Lipschitz continuous. The requirement  $S''(x(z)) \neq 0$  is only necessary (and sufficient) for formula (30) for  $\Lambda(z)$ . Moreover, supposing  $S'' > 0$  in a neighborhood of the minimum of  $S$ , then both  $\Sigma(z)$  and  $\Lambda(z)$  are well-defined in a neighborhood of  $z = 1$ .

We can now prove now that  $\Sigma, \Lambda$  defined as in (28, 30) satisfy the semiclassical PDEs (26,27) provided  $S, L$  satisfy the semiclassical PDEs (24,25).

**Theorem 6.** Let  $S(x, t), L(x, t), t \in [0, T[$  be solutions of equations (24,25) satisfying the hypotheses of Theorem 5 for all  $t$ 's. Let moreover  $\Gamma(z, t) \equiv \sum_k e^{-nS(\frac{k}{n}, t)} L(\frac{k}{n}, t)$ .

Then  $\Sigma(z, t) = \lim_{n \rightarrow \infty} \frac{\log \Gamma(z, t)}{n}$  exists and satisfies equations (26) for any  $z > 0$ . Moreover for any  $e^{S_x(0, t)} < z < e^{S_x(1, t)}$  then

$$\Gamma(z, t) \sim \sqrt{2\pi n} e^{n\Sigma(z, t)} \Lambda(z, t)$$

where  $\Lambda(z, t)$  satisfies (27).



*Proof.* By Theorem 5,  $\Sigma$  is the (restricted) Legendre-Fenchel transform of  $S$  evaluated at  $\ln z$ . It means that if  $\tilde{\Sigma}(y, t) = \Sigma(e^y, t)$  and  $y(x, t) = S_x(x, t)$  then

$$S(x, t) + \tilde{\Sigma}(y(x, t), t) = xy(x, t) .$$

Differentiating by  $t$ , we get

$$S_t + \Sigma_t = y_t(x - \tilde{\Sigma}_y(y(x, t), t)) .$$

Since  $x = \tilde{\Sigma}_y(y(x, t), t)$  ( $x, y$  are the conjugate variables of Legendre transform) then

$$\tilde{\Sigma}_t(y, t) - H(\tilde{\Sigma}_y, y) = 0 \text{ or equivalently } \Sigma_t(z, t) - H(z\Sigma_z, \ln z) = 0 .$$

A simple computation shows that  $-H(zq, \ln z) = \Theta(z, q)$ , for any  $z, q$ .

The proof that  $\Lambda$  satisfies the transport equation can be given following the same ideas but requires a more detailed description of the Hamilton-Jacobi theory. This goes beyond the scope of the present paper. However, since also the  $x$  and  $p$  representations in semi-classical quantum mechanics are related by the Legendre-Fenchel transform, then the proof can be derived, without any essential modification, from the proof of Theorem 5.3 in [9].  $\square$

Using the semiclassical equations for  $\Gamma(z)$ , we can show that the semiclassical dynamics conserves the total probability.

**Theorem 7.** *Let  $S(x, t), L(x, t), t \in [0, T[$  be solutions of equations (24, 25) satisfying the hypotheses of Theorem 5 for all  $t$ 's. Then*

$$\sum_{k=0}^n e^{-nS(\frac{k}{n}, t)} L(\frac{k}{n}, t) \sim \sum_{k=0}^n e^{-nS(\frac{k}{n}, 0)} L(\frac{k}{n}, 0), \quad \forall t \in [0, T[ . \quad (32)$$

*Proof.* We first observe that after Theorem 5,  $\sum_{k=0}^n e^{-nS(\frac{k}{n}, t)} L(\frac{k}{n}, t) \sim e^{n\Sigma(1, t)} \Lambda(1, t)$ . To prove the thesis it is sufficient to show that  $\Sigma(1, t)$  and  $\Lambda(1, t)$  are constant in time. We do that by means of the method of characteristics:

On the solution of the system of ODEs

$$\dot{z} = \partial_q \Theta(z, q), \dot{q} = -\partial_z \Theta(z, q), q(0) = \Sigma_z(z, 0)$$

then

$$\begin{aligned} \Sigma(z(t)) &= \Sigma(z(0)) + \int_0^t \partial_q \Theta(z(s), q(s)) q(s) ds \\ \Lambda(z(s)) &= \Lambda(z(0)) - \int_0^t \left( \frac{1}{2} \partial_q^2 \Theta(z(s), q(s)) \Sigma_{zz}(z(s)) + \beta(-z(s) + z^2(s)) \Sigma_z(z(s)) \right) ds . \end{aligned}$$

Since  $\dot{z} = 0$  if  $z = 0$  then the characteristic starting at  $z = 0$  will stay in  $z = 0$  for all  $t$ . Moreover, the integrals defining  $S, L$  vanish for all  $t$  as the integrands vanish identically at  $z = 0$ . Therefore  $\Sigma(1, t) = \Sigma(1, 0), \Lambda(1, t) = \Lambda(1, 0)$ .  $\square$

**Remark.** *Also in this Theorem we could relax the hypothesis. The Theorem holds, with a slightly more complex proof, if we just ask that  $S''(x, 0)$  and  $L(x, 0)$  do not vanish in a neighborhood of the global minimum of  $S(x, 0)$ .*

### An apparent paradox concerning the meta-stable state of SIS model

Assuming  $\frac{\beta}{\alpha} > 0$ , the SIS model admits a quasi-stationary or meta-stable state  $p^*$ , corresponding to an exponentially small eigenvalue of the transition matrix of the Markov chain (23), see [14] and references therein.

In the semiclassical regime and considering the probability distribution picture, the meta-stable state corresponds to a non-trivial stationary solution  $S^*$  of the Hamilton-Jacobi equation (24). This in turn corresponds to a zero-energy level-curve of the Hamiltonian as clearly  $S_t^* = 0$  if and only if  $H(x, S_x^*(x)) = 0$ . Explicitly [14]

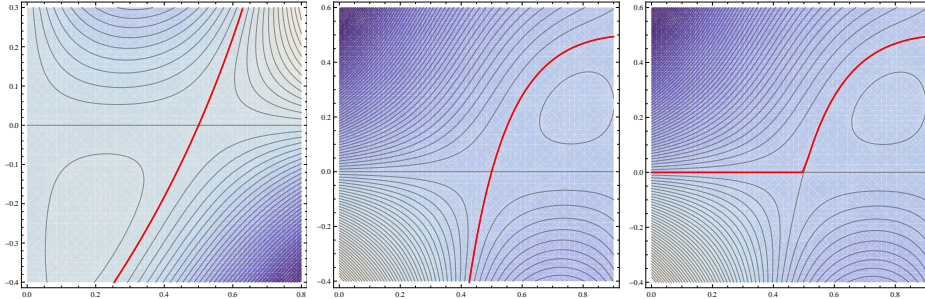
$$S^*(x) = q_x^*(x), \quad q^*(x) = \log \frac{\beta(1-x)}{\alpha} \quad (33)$$

Surprisingly, in the generating function picture there is no non-trivial smooth zero-energy level-curve of the Hamiltonian  $\Theta(z, Q^*(z))$  that satisfies the necessary condition  $Q^*(z) \geq 0$ , corresponding to the requirement  $p_k \geq 0, \forall k$ . In fact the only non-trivial smooth energy-level curve of the Hamiltonian is  $\frac{-\alpha + \beta z}{\beta z^2}$  that tends to  $-\infty$  as  $z \rightarrow 0^+$ . This seems to contradict Theorem 6, after which any stationary solution to (24) corresponds to a stationary solution of (26).

The solution of this apparent paradox comes from Theorem 5. After this Theorem, we know that  $\Sigma^*$  is not smooth even if  $S^*$  is smooth as the second derivative of  $\Sigma^*$  is discontinuous at  $z = e^{q^*(0)}, z = e^{-q^*(1)}$  (in this case  $e^{-q^*(1)} = +\infty$ ). This is because  $\Sigma^*$  is the restricted Legendre-Fenchel transform of  $S^*$ , formula (28). In fact, given  $S^*$  as above and using formula (28), we obtain

$$\Sigma^*(z) = Q_z^*(z), \quad Q^*(z) = 0 \text{ if } z < \frac{\alpha}{\beta}, \frac{-\alpha + \beta z}{\beta z^2} \text{ otherwise.} \quad (34)$$

$Q^*(z)$  is thus the union of two branches of two different smooth zero-energy level-curves of  $\Theta(z, q)$ , the trivial curve for  $z < \frac{\beta}{\alpha}$  and the non-trivial one for  $z \geq \frac{\beta}{\alpha}$ .



(c) Level curves of  $H(x, q)$ . The thick line is the derivative of the non-trivial stationary solution (33).  
(d) Level curves of  $\Theta(z, q)$ . The thick line is the derivative of the unphysical stationary solution.  
(e) Level curves of  $\Theta(z, q)$ . The thick line is the derivative of the correct (non-smooth) stationary solution  $Q^*(z)$  (34).

## 3 Concluding Remarks

We have analyzed the series  $I(n, \alpha)$  and shown that its asymptotic behaviour can be effectively computed for all values of  $\alpha$ . Most of the proofs we have given are

based on the comparison of the given series with a standard exponential or Gaussian series. On the other hand, we showed in the proof of Theorem 2 that it is possible to compute the asymptotic behaviour of the series by comparing it with the integral  $\mathcal{I}(n)$ . We did that by means of the Euler-McLaurin summation formula. As a consequence, we obtained two different ways of dealing with the series  $I(n, \alpha)$ .

The same methods we use allow to deal with a number of variations of the original problem. For example, in this work we have chosen to consider only functions  $f$  such that the global minimum is not-degenerate, that is either  $f'(0) > 0$  or  $f''(x_0) > 0$ . However, degenerate cases can be easily dealt along the lines of this work.

Also multidimensional series like

$$\sum_{k_1, \dots, k_m} e^{-nf(\frac{k_1}{n}, \dots, \frac{k_m}{n})} g(\frac{k_1}{n}, \dots, \frac{k_m}{n})$$

are amenable to the same analysis.

For what concerns the application to the semiclassical limit of population biology, we stick to the SIS model. As it was already noticed, our results in this respect can be extended with few or no modifications at all to many other models of population biology admitting a semiclassical limit.

In the impossibility of tackling the seemingly endless possible variations of the Laplace's method and its applications, we believe we have furnished the interested reader enough instruments to tackle some of the possible generalizations.

We conclude the paper with two interesting open problems.

The first problem is the asymptotic behaviour of the generating function for  $z$  not real and positive. For any  $f, g$ , the generating function can be cast into a series of the kind  $I(n, \alpha = 1)$

$$\Gamma(z) = \sum_{k=0}^n e^{-n\tilde{f}(\frac{k}{n})} g(\frac{k}{n}), \quad \tilde{f}(x) = f(x) - x(\ln|z| + i \arg z)$$

but if  $z$  is not positive,  $\tilde{f}$  is not real. Since the leading contributions are the ones close to the global maximum of  $|e^{-n\tilde{f}(\frac{k}{n})}|$ , that is close to the minimum point  $x(z)$  of  $Re\tilde{f}$ , we are led to approximate  $\Gamma(z)$  by the following Gaussian series with an imaginary linear term

$$e^{-n\tilde{f}(x(z))} \sum_k e^{-\frac{f''(x(z))}{2} \frac{(k-nx(z))^2 + in \arg z k}{n}} \sim e^{-nf(x(z))} e^{-\frac{n}{2f''(x(z))} \arg^2 z + in \arg z x(z)}.$$

The latter result stems from the Poisson summation formula applied to the series.

If  $\arg z$  is not real and positive, the latter series is thus exponentially small and even smaller than (the estimate of) the error term generated by neglecting contribution outside the maximum of  $|e^{-n\tilde{f}(\frac{k}{n})}|$ , which is - after the proof of Theorem 1-  $e^{-n\tilde{f}(x(z))} O(e^{-\frac{f''(x_0)}{2} n^{1-\beta}})$ , for any  $0 < \beta < \frac{1}{2}$ . Therefore we can conclude that  $\Gamma(z)$  is exponentially small relative to  $\Gamma(|z|)$  if  $z \neq |z|$ , but we do not know its precise asymptotic behaviour.

The second problem, whose solution would solve the first one in case  $f, g$  are analytic, is the steepest-descent method for the series  $I(n)$ . Let in fact  $f, g$  be analytic (not real) functions and suppose  $[0, \infty[$  can be deformed into a path of steepest descent for  $f$ . We can then compute  $\mathcal{I}(n)$  by the method of steepest descent.

However, does  $I(n) \sim \mathcal{I}(n)$  if  $\mathcal{I}(n)$  is computed by deforming the integration path? Unfortunately, the Euler-McLaurin formula (17) we use to estimate the difference between the series and the integral, does not allow to consider deformations of the integration contour because the Bernoulli functions are **not** analytic.

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